

Anhydromethylenecitric acid
144-16-1 | DTXSID60162592

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 154 °C

Global applicability domain: Inside

Local applicability domain index: 4.17e-01

Confidence level: 3.92e-01

Nearest Neighbors from the Training Set

Image not found

Butanoic acid, 4,4'-dioxybis[4-oxo-

Measured: 127

Predicted: 134

Image not found

Sulfonyldiacetic acid

Measured: 182

Predicted: 175

Image not found

Acetic acid, sulfo-

Measured: 85.0

Predicted: 104

Image not found

Chelidonic acid

Measured: 262

Predicted: 241

Image not found

alpha-Ketoglutaric acid

Measured: 116

Predicted: 160